

Gauge fields in graphene with nonuniform elastic deformations: A quantum field theory approach

Enrique Arias,¹ Alexis R. Hernández,² and Caio Lewenkopf³

¹*Instituto Politécnico, Universidade do Estado do Rio de Janeiro, 28625-570 Nova Friburgo, Brazil*

²*Instituto de Física, Universidade Federal do Rio de Janeiro, 21941-972 Rio de Janeiro, Brazil*

³*Instituto de Física, Universidade Federal Fluminense, 24210-346 Niterói, Brazil*

We investigate the low energy continuum limit theory for electrons in a graphene sheet under strain. We use the quantum field theory in curved spaces to analyze the effect of the system deformations into an effective gauge field. We study both in-plane and out-of-plane deformations and obtain a closed expression for the effective gauge field due to arbitrary nonuniform sheet deformations. The obtained results reveal a remarkable relation between the local-pseudo magnetic field and the Riemann curvature, so far overlooked.

PACS numbers: 73.22.Pr, 04.62.+v

I. INTRODUCTION

One of the most active research topics in graphene, as well as in other 2D materials, is the study of the interplay between their electronic and mechanical properties^{1–5}. Among the most remarkable results the possibility of using strain to generate large effective magnetic fields, with considerable effects on the electronic dynamics, has attracted a lot of attention^{6–8}. These results triggered several interesting strain engineering proposals, such as the use of strain for quantum electronic pumping^{9,10}, generation of pure bulk valley currents¹¹, and for confining electrons^{12,13}, to name a few.

There are two main theoretical approaches that cast strain/deformation induced modifications in the electronic properties of graphene monolayers in terms of effective gauge fields. The most standard one^{14–19} is based on the low-energy continuum limit of a tight-binding model that accounts for the displacements of the carbon atoms in a strained graphene sheet. This approach has been successful in explaining the local density of states inferred by scanning probe spectroscopy experiments in graphene nanobubbles^{20,21}. In contrast, to be consistent with transport experiments^{23,24}, the pseudo-magnetic fields have to be renormalized^{14,22}. Recent studies have further developed the theory showing the modifications in the effective theory due to the non-Bravais nature of the graphene primitive unit cell²² and the effects of deformations in the structure of the reciprocal space²⁵.

The second approach is based on the quantum field theory in curved spaces^{26,27}. It starts with the low-energy effective Dirac equation for graphene²⁸ and, by considering a curved space metric, obtains geometry-induced gauge fields^{29,30}. This theory was the first to predict a space-dependent Fermi velocity, that has been experimentally confirmed³¹. It has been recently shown³² that this approach can be extended beyond the continuum limit by using discrete differential geometry. The effective theory in curve spaces has also fostered interesting research in materials other than graphene^{33,34}.

The current theoretical status^{17,18} is that there is no unified approach that combines elasticity theory with the continuum limit of the corresponding tight-binding approximation¹⁶ and the quantum field theory in curved geometry (or geometrical approach)^{29,30}. Symmetry arguments¹⁷ indicate that there is room for improving both approaches. With this motivation our study focuses on further developing the geometric approach.

In this paper we advance the quantum field theory approach put forward in the seminal works of Vozmediano and collaborators^{29,30}, that addressed a case with a simple geometry, namely, a Gaussian bump deformation. We derive a general expression for the pseudo-magnetic field for an arbitrary nonuniform graphene surface deformation. By restricting our analysis to the case of out-of-plane lattice deformations, we are able to express the pseudo-magnetic field in a simple analytical form. This result reveals a remarkable relation between the pseudo-magnetic field and the Riemann curvature.

We further generalize these findings for the realistic case that combines in-plane and out-of-plane deformations by incorporating elements of elasticity theory³⁵. Here it is still possible to solve the problem and we can numerically verify that the relation between the pseudo-magnetic field and the scalar curvature holds. Unfortunately, the expressions for the gauge field induced by an arbitrary strain become very lengthy and not particularly insightful. For this reason, we use the simple Gaussian bump deformation to illustrate our results.

This paper is organized as follows. In Sec. II we review the theory of Dirac fermions in flat and curved spaces. In Sec. III we use this formalism to model the wave equation of quasi particles in rippled graphene. Next, we introduce a parameterization for a surface with an arbitrary curvature. By correctly defining the pseudo-magnetic field, we find a connection between the graphene curvature and the induced pseudo-magnetic field. In Sec. IV we discuss the local plane frame associated to a given point in the curved surface that has been used by some authors^{36,37} and show that the identification of the gauge field in this position-dependent frame leads to an incorrect as-

assessment of the pseudo-magnetic field. We present our conclusions in Sec. V.

II. DIRAC EQUATION IN CURVED SPACE

In this Section we briefly review the formalism of the Dirac equation in flat and curved spacetimes, paying particular attention to the technical issues most directly related to our study.

The flat spacetime points are denoted by $X = (T, \mathbf{X})$ whose components have *flat* indices denoted by the greek letters $\{\alpha, \beta, \delta, \dots\}$. The Dirac equation in the flat Minkowski spacetime is written as²⁷

$$(i\gamma^\alpha \partial_\alpha + m)\psi(X) = 0, \quad (1)$$

where γ^α are the usual Dirac matrices and $\partial_\alpha = \partial/\partial X^\alpha$. Since we work with differentiable functions the derivatives do commute, $[\partial_\alpha, \partial_\beta] = 0$.

In the presence of a gravitational field, Eq. (1) needs to be modified to account for a spacetime structure. In this case, the curved spacetime points are denoted by χ whose *curved* components we designate by the greek letters $\{\mu, \nu, \kappa, \dots\}$. The standard procedure for tensor (bosonic) fields is to realize the minimal coupling of the field with gravity by substituting the Minkowski spacetime metric tensor $\eta_{\alpha\beta}$ by the general Riemannian metric $g_{\mu\nu}$ and by the replacing of the usual derivative ∂_α by the covariant derivative ∇_μ . For spinorial (fermionic) fields this procedure is inadequate, due to the lack of a spinorial covariant derivative in terms of the metric. To correctly account for the coupling of the spinor with the curved spacetime one uses the vierbeins formalism^{26,27}.

The equivalence principle, that is the basis of the geometric theory of gravitation, states that one can not locally distinguish between a real gravitational field and the effects caused by a non-inertial reference frame³⁸. This implies that in the neighborhood \mathcal{X} of any given point χ_p in curved spacetime, one can find a local reference frame $\{\xi_\chi^a\}$ such that all the effects of gravity vanish.

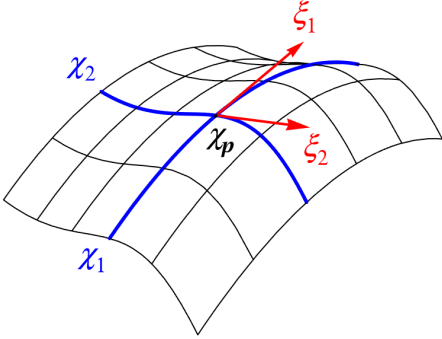


FIG. 1. Illustration of a curved surface: (χ_1, χ_2) correspond to global-curved coordinates and (ξ_1, ξ_2) to local-flat coordinates taken at a given point χ_p .

This local-flat space has the Minkowski metric η_{ab} and the distance between infinitesimally close points is $ds^2 = \eta_{ab} d\xi_\chi^a d\xi_\chi^b$. Near the point χ_p the same distance, given in terms of the curved coordinates, is $ds^2 = g_{\mu\nu} d\chi^\mu d\chi^\nu$. By comparing these expressions and considering that ξ_χ^a are local functions of χ_p , one concludes that

$$g_{\mu\nu}(\chi_p) = \eta_{ab} e_\mu^a(\chi_p) e_\nu^b(\chi_p), \quad (2)$$

where $e_\mu^a(\chi_p)$ are the so-called vierbeins, defined as^{26,27}

$$e_\mu^a(\chi_p) = \left. \frac{\partial \xi_\chi^a(\chi)}{\partial \chi^\mu} \right|_{\chi=\chi_p}. \quad (3)$$

The inverse vierbeins read $e^\mu_a = g^{\mu\nu} \eta_{ab} e_\nu^b$ and satisfy $g^{\mu\nu} = \eta^{ab} e^\mu_a e^\nu_b$. Note that these definitions are local.

In summary, in this paper we define three coordinate systems: (i) The global-flat Minkowski space with coordinates X , and component indices (α, β, \dots) ; (ii) The global-curved space with coordinates χ labeled by (μ, ν, \dots) ; (iii) The local-flat position dependent reference system with coordinates ξ and local-flat indices (a, b, \dots) .

The vierbeins are operators that transform quantities in the global-curved space to their corresponding local-flat counterparts. For example, one can find the curved version of the Dirac matrices, γ^μ , by contracting the flat gamma matrices γ^a with the vierbeins, namely

$$\gamma^\mu = e^\mu_a \gamma^a. \quad (4)$$

It can be verified that these matrices satisfy the generalized Clifford algebra in the curved spacetime $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$. Also, the covariant derivative ∇_μ of a spinorial field can now be properly defined as

$$\nabla_\mu \psi = (\partial_\mu + \Omega_\mu) \psi, \quad (5)$$

where Ω_μ is the so called spin connection, defined by

$$\Omega_\mu = \frac{1}{2} \omega_{\mu ab} \Sigma^{ab}, \quad (6)$$

with

$$\omega_{\mu ab} = e^\nu_a \nabla_\mu e_{\nu b} - e^\nu_b \nabla_\mu e_{\nu a}. \quad (7)$$

The covariant derivatives of the vierbeins read $\nabla_\mu e_{\nu a} = \partial_\mu e_{\nu a} - \Gamma_{\mu\nu}^\kappa e_{\kappa a}$ and the affine connections $\Gamma_{\mu\nu}^\kappa$ are the usual Christoffel symbols²⁶. The operators $\Sigma^{\alpha\beta}$ are the generators of the Lorentz group in the spinorial space, namely, $\Sigma^{\alpha\beta} = [\gamma^\alpha, \gamma^\beta]/4$.

Hence, the Dirac equation in a curved spacetime is given by

$$(i\gamma^\mu \nabla_\mu + m) \psi(\chi) = 0. \quad (8)$$

The covariant derivative, given by Eq. (5), allows one to interpret Ω_μ as an effective gauge field induced by the space curvature^{29,30}. The analysis of the pseudo-magnetic fields associated to Ω_μ is the main focus of this study.

We note that the space dependence of γ^μ gives rise to another important effect^{29,30}, namely, the renormalization of the electron velocity, called Fermi velocity v_F in the graphene literature. Our analysis reproduces the same effects showed Refs. 29 and 30 for the spacial dependence of v_F .

In summary, by knowing all the geometric objects associated to a given spacetime, one can establish the influence of the space curvature on the dynamics of the particles in that space. In the following Section we describe how to find the general geometric properties of an arbitrary curved graphene sheet. We then identify and discuss the correct pseudo-magnetic field generated by the corrugations.

III. APPLICATION TO CURVED GRAPHENE

We now adapt the results of Sec. II to describe the dynamics of electrons in rippled graphene by coupling a quenched curved background to the quasi-particle wave function. The procedure we present follows the ideas put forward by Vozmediano and collaborators²⁹ and generalizes their results to arbitrary sheet profiles. To that end, we have found a way to properly treat the gauge invariance associated to arbitrary curved spaces. This allowed us to identify a remarkable relation between the pseudo-magnetic field and the Riemann curvature. This relation implies that our results are manifestly gauge invariant, in distinction to previous studies.

Following the outline presented in Sec II, we describe the dynamics of electrons constrained to propagate in a two-dimensional curved surface by finding the metric, the vierbeins, the affine connection, and the spin connection associated to it.

A. Out-of-plane deformations

The geometry of a rippled two-dimensional surface can be parametrized by the function $z = h(x, y)$, where h represents the out of plane deviation from the flat surface $z = 0$. In the notation introduced in the previous section, $h(\chi)$ is the surface height at the position $\chi = (x, y)$. Since the coordinates (x, y) parameterize the curved surface, in general the intersection of the plane defined by a constant x (or y) with the surface $h(x, y)$ is not a straight line. Further, these curvilinear coordinates do not need to be orthogonal on the surface.

The square distance between two infinitesimally close points on the curved surface is given by

$$ds^2 = [1 + (\partial_x h)^2] dx^2 + [1 + (\partial_y h)^2] dy^2 + 2(\partial_x h)(\partial_y h) dx dy. \quad (9)$$

We write Eq. (9) as $ds^2 = g_{\mu\nu} d\chi^\mu d\chi^\nu$. For notation convenience, to establish a clear difference between curved and flat indices, we call (χ^x, χ^y) *curved coordinates*,

whose “curved” indices are denoted by $\mu = \{x, y\}$. In terms of the curved coordinates the metric on the manifold reads

$$g_{\mu\nu} = \begin{pmatrix} 1 + h_x^2 & h_x h_y \\ h_x h_y & 1 + h_y^2 \end{pmatrix}, \quad (10)$$

where we introduce the shorthand notation $h_\mu = \partial_\mu h$. It is convenient, for later use, to write $g_{\mu\nu}$ in a compact form as

$$g_{\mu\nu} = \delta_{\mu\nu} + h_\mu h_\nu. \quad (11)$$

As already discussed, locally at each point χ of the curved surface, the manifold can be seen as flat, and there exists a local coordinate system such that in a small region \mathcal{X} , near the point χ , the metric is Euclidean. We denote this local flat coordinates by $\xi_\chi^a = \xi_\chi^a(\chi)$, with “local-flat” indices $a = \{1, 2\}$. In terms of the local-flat coordinates, the square distance between two points is given by $ds^2 = \delta_{ab} d\xi_\chi^a d\xi_\chi^b$. Comparing this expression with $ds^2 = g_{\mu\nu} d\chi^\mu d\chi^\nu$ defined above, we find the relation between both metrics, namely

$$g_{\mu\nu}(\chi) = \delta_{ab} e_\mu^a(\chi) e_\nu^b(\chi). \quad (12)$$

Due to the symmetry $g_{\mu\nu} = g_{\nu\mu}$, Eq. (12) gives three independent relations to find the vectors $e_\mu^1 = (e_x^1, e_y^1)$ and $e_\mu^2 = (e_x^2, e_y^2)$. In this way, except for a single degree of freedom, the vierbeins are determined by the metric. It will be shown that this indetermination does not manifest in physical observables. By simple algebraic manipulation we obtain a general solution for the vierbeins, namely

$$e_\mu^a = \begin{pmatrix} \sqrt{1 + h_x^2} \cos \theta & \sqrt{1 + h_x^2} \sin \theta \\ \sqrt{1 + h_y^2} \cos \bar{\theta} & \sqrt{1 + h_y^2} \sin \bar{\theta} \end{pmatrix}, \quad (13)$$

where $\theta = \theta(x, y)$ is an arbitrary function related to the orientation of the local-flat coordinate axis at the point $\chi = (x, y)$. In Eq. (13) we also introduced $\bar{\theta}$, given by

$$\bar{\theta} = \theta + \arccos \left(\frac{h_x h_y}{\sqrt{(1 + h_y^2)(1 + h_x^2)}} \right). \quad (14)$$

Let us now calculate the inverse vierbeins, $e^\mu_a = g^{\mu\nu} \delta_{ab} e_\nu^b$. From Eq. (10) we obtain the inverse metric

$$g^{\mu\nu} = \frac{1}{1 + h_x^2 + h_y^2} \begin{pmatrix} 1 + h_y^2 & -h_x h_y \\ -h_x h_y & 1 + h_x^2 \end{pmatrix}. \quad (15)$$

or

$$g^{\mu\nu} = (\delta^{\mu\nu} + h_\mu^* h_\nu^*) / (1 + h_x^2 + h_y^2), \quad (16)$$

where we have introduced the dual $h_\mu^* = \varepsilon_{\mu\nu} h_\nu$, being $\varepsilon_{\mu\nu}$ the Levi-Civita tensor in two dimensions, *i.e.*, $\varepsilon_{12} =$

$-\varepsilon_{21} = 1$ and $\varepsilon_{11} = \varepsilon_{22} = 0$. By using Eqs. (13) and (15) we calculate the inverse vierbeins

$$e^\mu_a = \frac{1}{\sqrt{1+h_x^2+h_y^2}} \begin{pmatrix} \sqrt{1+h_y^2} \sin \bar{\theta} & -\sqrt{1+h_y^2} \cos \bar{\theta} \\ -\sqrt{1+h_x^2} \sin \theta & \sqrt{1+h_x^2} \cos \theta \end{pmatrix}. \quad (17)$$

Having defined the metric tensor and the vierbeins, we proceed to calculate the spin connection that relates the wave function of the Dirac field with the curved space geometry. First, we determine the vierbeins covariant derivatives which are expressed in terms of the affine connection. The affine connections coincide with the Christoffel's symbols in the case where the spacetime has a curvature but not a torsion³⁹. Effects of torsion have been studied in the context of topological defects⁴⁰, which are not within the scope of this paper. Hence,

$$\Gamma_{\mu\nu}^\kappa = \frac{1}{2} g^{\kappa\sigma} (\partial_\mu g_{\nu\sigma} + \partial_\nu g_{\mu\sigma} - \partial_\sigma g_{\mu\nu}). \quad (18)$$

By using Eqs. (11) and (16) we express the affine connection in terms of h , namely

$$\Gamma_{\mu\nu}^\kappa = \frac{h_{\mu\nu} h_\kappa}{1+h_x^2+h_y^2}, \quad (19)$$

where $h_{\mu\nu} = \partial_{\mu\nu}^2 h$.

Before we obtain the spin connection, it is instructive to present the curvature tensors associated to the surface. The Riemann curvature tensor is given by

$$R_{\mu\nu\rho}^\kappa = \partial_\mu \Gamma_{\nu\rho}^\kappa - \partial_\nu \Gamma_{\mu\rho}^\kappa + \Gamma_{\mu\sigma}^\kappa \Gamma_{\nu\rho}^\sigma - \Gamma_{\nu\sigma}^\kappa \Gamma_{\mu\rho}^\sigma, \quad (20)$$

while the scalar curvature of the surface reads

$$\mathcal{R} = R_{\kappa\mu\nu}^\kappa g^{\mu\nu}. \quad (21)$$

Hence, for the two-dimensional graphene surface with out-of-plane deformations the scalar curvature reads

$$\mathcal{R} = 2 \frac{h_{xx} h_{yy} - h_{xy}^2}{(1+h_x^2+h_y^2)^2}. \quad (22)$$

Let us now resume the calculation of the spin connection Ω_μ of the Dirac field for a general two-dimensional curved surface, defined by Eq. (6) in terms of the components $\omega_{\mu ab}$ ²⁶, given by Eq. (7). Due to the antisymmetry of the $\omega_{\mu ab}$ in its flat indices, the only non-zero component is $\omega_{\mu 12}$. One can identify the later with the effective gauge field induced by the curvature, and call $\mathcal{A}_\mu = \omega_{\mu 12}$ ²⁹.

After some algebra, we obtain that, for a general two-dimensional curved surface described by the function $h = h(x, y)$, the effective gauge field is given by

$$\mathcal{A}_\mu = \frac{1}{\sqrt{1+h_x^2+h_y^2}} \left(\frac{h_x h_{y\mu}}{1+h_y^2} - \frac{h_y h_{x\mu}}{1+h_x^2} \right) + \partial_\mu (\theta + \bar{\theta}). \quad (23)$$

The arbitrary angle $\theta = \theta(x, y)$ enters as a total derivative in the gauge field \mathcal{A}_μ and therefore does not affect the pseudo-magnetic field $\mathcal{B} = \text{rot} \mathcal{A}$, associated to \mathcal{A}_μ . Arbitrary independent rotations of the local-flat frames along the curved surface, do not change the pseudo-magnetic field and translate as the *gauge transformations* of the field \mathcal{A}_μ .

The formal definition of the curl operator in non-orthogonal curvilinear coordinates is

$$\mathcal{B} = \frac{1}{\sqrt{g}} \varepsilon^{\mu\nu} \nabla_\mu \mathcal{A}_\nu, \quad (24)$$

where $g = \det(g_{\mu\nu})$ and $\varepsilon^{\mu\nu}$ is the Levi-Civita symbol. By using the metric from Eq. (10) and the gauge field obtained in Eq. (23), we find that

$$\mathcal{B} = 2 \frac{h_{xx} h_{yy} - h_{xy}^2}{(1+h_x^2+h_y^2)^2}. \quad (25)$$

In two spacial dimensions the electromagnetic tensor becomes an anti-symmetric tensor of order three. This ensures that in two-dimensions the electric field is a vector, but the magnetic field has a single (scalar) component, perpendicular to the local-flat space associate to a given point in the deformed surface. Hence, based on invariance arguments, one can expect \mathcal{B} to be an arbitrary function of the scalar curvature, namely, $\mathcal{B} = F(\mathcal{R})$. A direct comparison between Eqs. (25) and (22) shows that the effective pseudo-magnetic field induced by ripples in graphene (in arbitrary units) is identical to the scalar curvature at each point of the surface

$$\mathcal{B} = \mathcal{R}. \quad (26)$$

The construction that leads to Eq. (25) and the above identity are the main findings of this paper.

We note that Eq. (25) generalizes the results presented in Ref. 30, where the case of a radial symmetric $h(x, y) = f(r)$ was studied. For this simple geometry, the surface is conveniently parameterized by polar coordinates (r, ϕ) . Here, our general expression for \mathcal{A}_μ , Eq. (23), reduces to the one found in Ref. 30. Using Eq. (25), we find

$$\mathcal{B} = \frac{2}{r} \frac{f' f''}{(1+f'^2)^2}. \quad (27)$$

In distinction to our approach, Ref. 30 obtains a pseudo-magnetic field in the z -direction (perpendicular to the undeformed graphene sheet). There, the pseudo-magnetic field is defined by $B_z = (1/r) \partial_r (r \mathcal{A}_\phi)$, which gives $B_z = (2/r) f' f'' (1+f'^2)^{-3/2}$. The discrepancy is due to the fact that Ref. 30 calculates B_z using the curl operator in flat polar coordinates while \mathcal{A}_ϕ is expressed in curved coordinates. Since the normal to the graphene surface is $\mathbf{n} = (-h_x, -h_y, 1)/(1+h_x^2+h_y^2)^{1/2}$, our pseudo-magnetic field projected in the z -direction is $\mathcal{B}/(1+f'^2)^{1/2}$. Hence, the results are not consistent.

This difference prevents one to identify the pseudo-magnetic field with the scalar curvature, but is unlikely to impact on the analysis of experiments, where the value of $\text{rms}(f')$ is typically smaller than 0.1^{24,41,42}.

B. The general case: in-plane and out-of-plane deformations

Here we analyze the general case of out-of-plane combined with in-plane deformations. Now the infinitesimal distance between points at the corrugated surface is $ds^2 = g_{\mu\nu}d\chi^\mu d\chi^\nu$, where the metric is expressed as

$$g_{\mu\nu} = \delta_{\mu\nu} + 2u_{\mu\nu}, \quad (28)$$

in terms of the deformation tensor, defined by the in-plane displacement vectors $u_\mu = u_\mu(x, y)$ and by the out-of-plane deformations $h(x, y)$ as follows

$$u_{\mu\nu} = \frac{1}{2}(\partial_\mu u_\nu + \partial_\nu u_\mu + 2h_\mu h_\nu). \quad (29)$$

Equations (28) and (29) are identical to those used in elasticity theory³⁵. This similarity will be explored in the next section to obtain material dependent expressions for the displacement vector components $u_\mu(x, y)$ in terms of the sheet topography $h(x, y)$.

Having defined the metric of the two-dimensional graphene surface we can proceed as before. The derivation has the same structure, the differences appear in the explicit expressions for the vierbeins, which are modified by the new physical ingredients. The general metric is

$$g_{\mu\nu} = \begin{pmatrix} g_{xx} & g_{xy} \\ g_{xy} & g_{yy} \end{pmatrix}. \quad (30)$$

The solutions for the vierbeins read

$$e_\mu^a = \begin{pmatrix} \sqrt{g_{xx}} \cos \theta & \sqrt{g_{xx}} \sin \theta \\ \sqrt{g_{yy}} \cos \theta & \sqrt{g_{yy}} \sin \theta \end{pmatrix}. \quad (31)$$

It can be checked that they satisfy $g_{\mu\nu} = \delta_{ab} e_\mu^a e_\nu^b$. As before, in Eq. (31), the variable $\theta = \theta(x, y)$ is an arbitrary angle related to the freedom of the orientation axes of local flat frames at point χ . Here we define

$$\bar{\theta} = \theta + \arccos\left(\frac{g_{xy}}{\sqrt{g_{xx}g_{yy}}}\right). \quad (32)$$

To calculate the inverse vierbeins $e^\mu_a = g^{\mu\nu} \delta_{ab} e_\nu^b$, we need the inverse metric, namely

$$g^{\mu\nu} = \frac{1}{g} \begin{pmatrix} g_{yy} & -g_{xy} \\ -g_{xy} & g_{xx} \end{pmatrix}. \quad (33)$$

As a result, the inverse vierbeins are

$$e^\mu_a = \frac{1}{\sqrt{g}} \begin{pmatrix} \sqrt{g_{yy}} \sin \bar{\theta} & -\sqrt{g_{yy}} \cos \bar{\theta} \\ -\sqrt{g_{xx}} \sin \theta & \sqrt{g_{xx}} \cos \theta \end{pmatrix}. \quad (34)$$

Given \mathbf{u} and h , these elements allow us to evaluate the effective pseudo-magnetic field, \mathcal{B} , generated by a combinations of out-of-plane and in-plane corrugations in graphene. However, in distinction to the out-of-plane case, the problem does not have a simple analytical solution. We still verify that $\mathcal{B} = \mathcal{R}$ for a number of different models for strains and corrugations. In the forthcoming section we illustrate our results by analysing the case of a simple geometry $h(x, y)$.

C. Application: Gaussian deformation in graphene

To construct the deformation tensor $u_{\mu\nu}$, Eq. (29), it is necessary to know both $h(x, y)$ and the displacement vector fields $u_\nu(x, y)$. The elasticity theory allows one to relate these quantities, as follows. We consider the simplified scenario where we neglect shear forces between the substrate and the two-dimensional material under analysis. We follow the procedure suggested by Guinea and collaborators¹⁶, namely, we assume that the system has a given system topography $h(x, y)$ and minimize the elastic energy by varying the in-plane degrees of freedom to obtain $\mathbf{u}(x, y)$.

The Hamiltonian corresponding to the elastic degrees of freedom reads¹⁶

$$\mathcal{H}_{\text{elastic}} = \int d\mathbf{r} \left\{ \frac{\lambda}{2} \left[\sum_{\nu} u_{\nu\nu}(\mathbf{r}) \right]^2 + \mu \sum_{\nu\nu'} [u_{\nu\nu'}(\mathbf{r})]^2 \right\}, \quad (35)$$

where μ and λ are the Lamé parameters of the material, which can be inferred from experiments and/or from first principle calculations. In this paper we use the parameter values proposed in Ref. 43, namely, $\mu = 103.89 \text{ J/m}^2$ and $\lambda = 15.55 \text{ J/m}^2$.

This construction adds important elements to the purely geometric theory developed in Sec. III A. Here, one needs the material parameters to establish a link between the in-plane displacements u_ν and the topography h . We stress that this procedure is still a geometric approach, since it incorporates u_ν in the metric. This is different from the standard tight-binding theory, where the metric is entirely absent.

Let us now calculate the in-plane displacement $\mathbf{u}(x, y)$ for the case of Gaussian deformation, namely, $h(\mathbf{r}) = h_0 \exp(-r^2/\sigma^2)$. This simple geometry allows for an analytical solution. The minimization of $\mathcal{H}_{\text{elastic}}$ renders a set of differential equations that are solved in the momentum space¹⁶. The result is

$$\mathbf{u}(\mathbf{k}) = -ih_0^2 e^{-\frac{1}{8}k^2\sigma^2} \frac{k^2\sigma^2(\lambda + 2\mu) - 8(\lambda + \mu)}{32k^2(\lambda + 2\mu)} \mathbf{k}, \quad (36)$$

which, in configuration space, reads

$$\mathbf{u}(\mathbf{r}) = \sqrt{\frac{\pi}{2}} h_0^2 \mathbf{r} e^{-2r^2/\sigma^2} \times \frac{-2r^2(\lambda + 2\mu) + \sigma^2(\lambda + \mu) (e^{2r^2/\sigma^2} - 1)}{2r^2\sigma^2(\lambda + 2\mu)}. \quad (37)$$

The vector field representing the in-plane displacements $\mathbf{u}(x, y)$ is shown in Fig. 2.

The in-plane displacement \mathbf{u} changes the strain tensor $u_{\mu\nu}$, the metric, and consequently the local pseudo-magnetic field $\mathcal{B}_{\text{relax}}$. Unfortunately, even for a topography as simple as that of a Gaussian bump, the analytical expression for $\mathcal{B}_{\text{relax}}$ becomes rather lengthy and is not

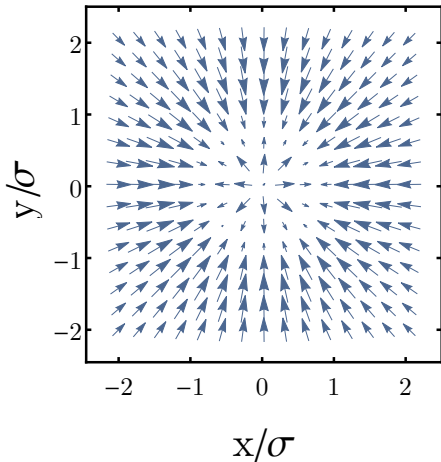


FIG. 2. Vector field representing the in-plane displacement $\mathbf{u}(x, y)$ for a Gaussian bump with $h_0 = 1$ nm and $\sigma = 5$ nm. The arrows represent the magnitude and direction of \mathbf{u} (in arbitrary units).

particularly insightful. Hence, we evaluate $\mathcal{B}_{\text{relax}}$ numerically, following the steps described in Sec. III B.

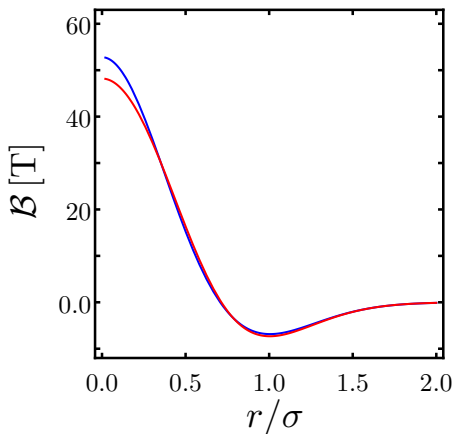


FIG. 3. (Color online) Pseudo-magnetic field \mathcal{B} as a function of r corresponding to a Gaussian bump deformation with $h_0 = 1$ nm and $\sigma = 5$ nm. The blue line represents the case without in-plane relaxation, while the red curve accounts for both out-of-plane and in-plane deformations.

The physical picture that emerges is that the in-plane relaxation reduces the mechanical stress, diminishing the magnitude of the pseudo-magnetic field, as shown in Fig. 3. We find that the in-plane relaxation corrections to \mathcal{B} are small for ripples usually found in graphene deposited on standard substrates, where $h_0 \ll \sigma$ ^{41,42}. They become significant in situations where h_0 is comparable with σ , such as in the case of nanobubbles²⁰. In Fig. 4 we plot a measure of the in-plane deformation contribution

to the pseudo-magnetic field, namely,

$$\Delta = \frac{\mathcal{B} - \mathcal{B}_{\text{relax}}}{\mathcal{B}_{\text{relax}}} \Big|_{\mathbf{r}=0}, \quad (38)$$

as a function of h_0/σ .

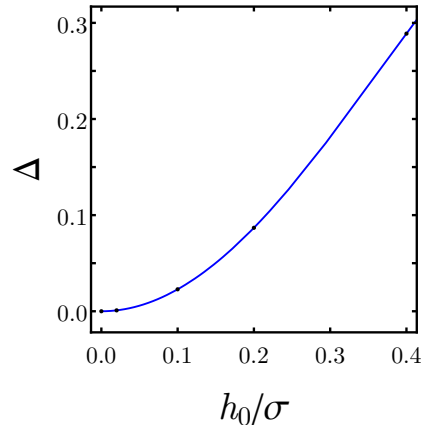


FIG. 4. Ratio Δ between the in-plane contribution $\mathcal{B} - \mathcal{B}_{\text{relax}}$ and the total pseudo-magnetic field $\mathcal{B}_{\text{relax}}$ at $\mathbf{r} = 0$, defined by Eq. (38), as a function of h_0/σ .

IV. GAUGE INVARIANCE AND THE LOCAL PLANE APPROXIMATION

In the previous sections we have studied the influence of a modified metric on the Dirac Hamiltonian. So far, despite some elaborate efforts^{36,44}, a unified picture conciliating this quantum field theory approach with the standard band structure theory has not been established. In this section we discuss some fundamental problems in constructing a bridge between these two approaches. From the practical point of view, as stressed in Ref. 36, while the geometric theory predicts a renormalization of the Fermi velocity, the elasticity approach does not. This issue was addressed in Ref. 36, where the authors analyze the local-flat Dirac equation starting from the global-curved one, namely

$$i\gamma^\mu(\partial_\mu + \Omega_\mu)\psi(\chi) = 0, \quad (39)$$

where γ^μ are the curved Dirac matrices $\gamma^\mu = \gamma^a e^\mu_a$. One can define the derivative with respect to the local-flat tangent space coordinates as

$$\partial_a = \frac{\partial}{\partial \xi^a_{\mathcal{X}}} e^\mu_a \partial_\mu. \quad (40)$$

The spin connection is given by $\Omega_\mu = \omega_{\mu 12} \Sigma^{12}$ with $\Sigma^{12} = [\gamma^1, \gamma^2]/4$. By using the representation of the

Dirac matrices for graphene

$$\gamma^0 = \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}; \gamma^1 = i \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix}; \gamma^2 = i \begin{pmatrix} \sigma_y & 0 \\ 0 & -\sigma_y \end{pmatrix}, \quad (41)$$

where σ_i are the usual Pauli matrices, one obtains $\gamma^a \Sigma^{12} = -\frac{1}{2} \varepsilon^{ab} \gamma^b$. Thus, the Dirac Hamiltonian, in the local-flat tangent space, reads

$$i\gamma^a(\partial_a + A_a)\psi(x) = 0, \quad (42)$$

where A_a has been associated³⁶ with a gauge potential defined by

$$A_a = \varepsilon_{ab} e_b^\mu \omega_{\mu 12}, \quad (43)$$

which originates the pseudo-magnetic field.

Despite being very appealing, this construction of a Dirac equation with a gauge potential in flat-tangent space, is problematic. First, the gauge potential A_a does not lead to a gauge invariant B -field. This statement is justified as follows: Let us assume we rotate the local-flat tangent space coordinates $\{\xi_\chi^a\}$, defined at every point of the surface $\chi(x, y)$, by an angle $\delta\theta(x, y)$. The curved gauge potential \mathcal{A}_μ of Eq. (23) and the local-flat potential A_a transform as

$$\delta\mathcal{A}_\mu = \partial_\mu(\delta\theta) \quad \text{and} \quad \delta A_a = \varepsilon_{ab} e_b^\mu \partial_\mu(\delta\theta). \quad (44)$$

One can see that these local rotations constitute a gauge transformation for the curved potential \mathcal{A}_μ and therefore the corresponding pseudo-magnetic field is gauge invariant. Gauge invariance is not preserved for A_a , since in the local-flat tangent space the pseudo-magnetic field given by $B = \varepsilon^{ab} \partial_a A_b$ depends explicitly on $\delta\theta$.

Secondly, the local-tangent space derivative ∂_a , Eq. (42), is not a standard derivative, since the commutator $[\partial_a, \partial_b]$ does not vanish, in general. We can show that

$$[\partial_a, \partial_b] = t_{ab}^c \partial_c, \quad (45)$$

being the *non-holonomicity coefficients*, t_{ab}^c , defined by

$$t_{ab}^c = (e_a^\mu \partial_\mu e_b^\nu - e_b^\mu \partial_\mu e_a^\nu) e_\nu^c. \quad (46)$$

This is different in the global-flat case, where $[\partial_\alpha, \partial_\beta] = 0$, as discussed after Eq. (1). Therefore, the local-flat Dirac equation Eq. (42) can not be mapped into the usual Dirac equation in flat space.

This problem remained unnoticed so far. Specifically Ref. 37 uses similar vierbeins as ours, but with the condition $e_x^2 = e_y^1$ to simplify the calculations. This choice implicitly fixes the gauge degree of freedom to be

$$\theta(x, y) = \arccos \left(\frac{h_y^2 + h_x^2 \sqrt{1 + h_x^2 + h_y^2}}{(h_x^2 + h_y^2) \sqrt{1 + h_x^2}} \right). \quad (47)$$

Due to this unphysical gauge dependence, the obtained pseudo-magnetic field is not unique.

V. CONCLUSIONS

In this paper we generalized the quantum field theory approach used to describe the low-energy electronic dynamics in rippled graphene. By considering a general two-dimensional curved graphene surface, we have properly identified the gauge transformations in that curved space. This lead us to define the effective gauge potential induced by the curvatures and to find an explicitly gauge invariant pseudo-magnetic field. We have found an equivalence between the pseudo-magnetic field induced by the ripples and the intrinsic scalar curvature of the general curved graphene surface. This remarkable relation, namely, $\mathcal{B} = \mathcal{R}$, has been overlooked so far and constitutes the main contribution of this paper.

We have extended these results to the realistic case where both out-of-plane and in-plane deformations are considered. We find that this generalization preserves the equivalence between the pseudo-magnetic field and the intrinsic scalar curvature. As an application, we have analyzed the specific case of a Gaussian bump deformation. We used the elasticity theory to write the deformation energy in terms of the strain tensor and few elastic material parameters. Following a minimization procedure¹⁶, we found an analytical relation between the displacement field the system topography for a simple geometry. We analyzed the magnitude of the in-plane contributions to the pseudo-magnetic field. We found that since the pseudo-magnetic field is exactly the surface scalar curvature, it will be modified by in-plane deformations, this is because these strains are not homogeneous nor uniform in space.

We have also discussed the local-flat tangent space approximation used in the literature to identify the effective gauge field induced in deformed graphene. We conclude that the identification of a Dirac equation in that position-dependent tangent space is problematic, since it can lead to unphysical gauge dependent results.

ACKNOWLEDGMENTS

We thank Tobias Micklitz, Nami Svaiter, Luis Durand, and Marco Moriconi for useful discussions. This work has been supported by the Brazilian funding agencies CAPES, CNPq, and FAPERJ.

- ¹ J. S. Bunch, A. M. van der Zande, S. S. Verbridge, I. W. Frank, D. M. Tanenbaum, J. M. Parpia, H. G. Craighead, and P. L. McEuen, *Science* **315**, 490 (2007).
- ² D. Garcia-Sanchez, A. M. van der Zande, A. S. Paulo, B. Lassagne, P. L. McEuen, and A. Bachtold, *Nano Lett.* **8**, 1399 (2008).
- ³ C. Chen, S. Rosenblatt, K. I. Bolotin, W. Kalb, P. Kim, I. Kymissis, H. L. Stormer, T. F. Heinz, and J. Hone, *Nature Nanotech.* **4**, 861 (2009).
- ⁴ A. Eichler, J. Moser, J. Chaste, M. Zdrojek, I. Wilson-Rae, and A. Bachtold, *Nature Nanotech.* **6**, 339 (2011).
- ⁵ G. W. Jones and V. M. Pereira, *New J. Phys.* **16**, 093044 (2014).
- ⁶ F. Guinea, M. I. Katsnelson, and A. K. Geim, *Nature Phys.* **6**, 30 (2009).
- ⁷ V. M. Pereira and A. H. Castro Neto, *Phys. Rev. Lett.* **103**, 046801 (2009).
- ⁸ T. Low, F. Guinea, and M. I. Katsnelson, *Phys. Rev. B* **83**, 195436 (2011).
- ⁹ E. Prada, P. San-Jose, and H. Schomerus, *Phys. Rev. B* **80**, 245414 (2009).
- ¹⁰ T. Low, Y. Jiang, M. I. Katsnelson, and F. Guinea, *Nano Lett.* **12**, 850 (2012).
- ¹¹ Y. Jiang, T. Low, K. Chang, M. I. Katsnelson, and F. Guinea, *Phys. Rev. Lett.* **110**, 046601 (2013).
- ¹² S. Zhu, Y. Huang, N. N. Klimov, D. B. Newell, N. B. Zhitenev, J. A. Strosio, S. D. Solares, and T. Li, *Phys. Rev. B* **90**, 075426 (2014).
- ¹³ R. Carrillo-Bastos, D. Faria, A. Latge, F. Mireles, and N. Sandler, *Phys. Rev. B* **90**, 041411(R) (2014).
- ¹⁴ H. Suzuura and T. Ando, *Phys. Rev. B* **65**, 235412 (2002).
- ¹⁵ J. L. Mañes, *Phys. Rev. B* **76**, 045430 (2007).
- ¹⁶ F. Guinea, B. Horovitz, and P. Le Doussal, *Phys. Rev. B* **77**, 205421 (2008).
- ¹⁷ J. L. Mañes, F. de Juan, M. Sturla, and M. A. H. Vozmediano, *Phys. Rev. B* **88**, 155405 (2013).
- ¹⁸ F. de Juan, J. L. Mañes, and M. A. H. Vozmediano, *Phys. Rev. B* **87**, 165131 (2013).
- ¹⁹ M. Ramezani Masir, D. Moldovan, and F. Peeters, *Solid State Commun.* **175-176**, 76 (2013).
- ²⁰ N. Levy, S. A. Burke, K. L. Meaker, M. Panlasigui, A. Zettl, F. Guinea, A. H. Castro Neto, and M. F. Crommie, *Science* **329**, 544 (2010).
- ²¹ N.-C. Yeh, M.-L. Teague, S. Yeom, B. L. Standley, R.-P. Wu, D. A. Boyd, and M. W. Bockrath, *Surface Science* **605**, 1649 (2011).
- ²² D. Midtvedt, C. H. Lewenkopf, and A. Croy, arXiv:1509.02365 (2015).
- ²³ M. B. Lundeberg and J. A. Folk, *Phys. Rev. Lett.* **105**, 146804 (2010).
- ²⁴ R. Burgos, J. Warnes, L. R. F. Lima, and C. Lewenkopf, *Phys. Rev. B* **91**, 115403 (2015).
- ²⁵ M. Oliva-Leyva and G. G. Naumis, *Phys. Rev. B* **88**, 085430 (2013).
- ²⁶ S. Weinberg, *Gravitation and Cosmology: Principles and Applications to the General Theory of Relativity* (Wiley and Sons, New York, 1972).
- ²⁷ N. D. Birrell and P. C. W. Davis, *Quantum Fields in Curved Space* (Cambridge University Press, Cambridge, 1982).
- ²⁸ G. W. Semenoff, *Phys. Rev. Lett.* **53**, 2449 (1984).
- ²⁹ M. A. H. Vozmediano, M. I. Katsnelson, and F. Guinea, *Phys. Rep.* **496**, 109 (2010).
- ³⁰ F. de Juan, A. Cortijo, and M. A. H. Vozmediano, *Phys. Rev. B* **76**, 165409 (2007).
- ³¹ H. Yan, Z.-D. Chu, W. Yan, M. Liu, L. Meng, M. Yang, Y. Fan, J. Wang, R.-F. Dou, Y. Zhang, Z. Liu, J.-C. Nie, and L. He, *Phys. Rev. B* **87**, 075405 (2013).
- ³² A. A. Pacheco Sanjuan, Z. Wang, H. Pour Imani, M. Vanevic, and S. Barraza-Lopez, *Phys. Rev. B* **89**, 121403(R) (2014).
- ³³ D. V. Khveshchenko, *EPL (Europhysics Letters)* **104**, 47002 (2013).
- ³⁴ G. E. Volovik and M. A. Zubkov, *Nucl. Phys. B* **881**, 514 (2014).
- ³⁵ L. D. Landau and E. M. Lifshitz, *Theory of elasticity*, 3rd ed. (Butterworth-Heinemann, Oxford, 1986).
- ³⁶ F. de Juan, M. Sturla, and M. A. H. Vozmediano, *Phys. Rev. Lett.* **108**, 227205 (2012).
- ³⁷ A. J. Chaves, T. Frederico, W. de Paula, and M. C. Santos, *J. Phys.: Condens. Matter* **26**, 1853301 (2014).
- ³⁸ P. Ramon, *Field Theory: A Modern Primer* (Addison-Wesley, New York, 1989).
- ³⁹ V. de Sabbata and M. Gasperini, *Introduction to Gravitation* (World Scientific, Singapore, 1985).
- ⁴⁰ F. de Juan, A. Cortijo, and M. A. H. Vozmediano, *Nucl. Phys. B* **828**, 625 (2009).
- ⁴¹ M. Ishigami, J. H. Chen, W. G. Cullen, M. S. Fuhrer, and E. D. Williams, *Nano Lett.* **7**, 1643 (2007).
- ⁴² V. Geringer, M. Liebmann, T. Echtermeyer, S. Runte, M. Schmidt, R. Rückamp, M. C. Lemme, and M. Morgenstern, *Phys. Rev. Lett.* **102**, 076102 (2009).
- ⁴³ J. Atalaya, A. Isacson, and J. M. Kinaret, *Nano Lett.* **8**, 4196 (2008).
- ⁴⁴ B. Yang, *Phys. Rev. B* **91**, 241403 (2015).